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Concerns with ENDF/B-VII Data Identified during Data Testing with MCNP5™

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To Be Presented at the 2005 mini-CSEWG Meeting
Oak Ridge National Laboratory July 13, 2005

The initial release of nuclear data for ENDF/B-VII is expected to occur in late 2005 or early 2006. Although data testing for that anticipated release has shown substantial improvement in overall agreement with integral benchmark results, it also has identified some problems that still need to be addressed. This presentation identifies specific areas for concern, including the unresolved resonance region for ^{235}U, fast and thermal cross sections for Th, fast cross sections for ^{237}Np and Cu, thermal cross sections for ^{233}U and ^{239}Pu, and the angular scattering distribution for ^{2}H.

Concerns with ENDF/B-VII Data Identified during Data Testing with MCNP5™

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Presented by
Robert C. Little

Presented at the 2005 mini-CSEWG Meeting
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IMPROVEMENTS PRODUCED BY INITIAL RELEASE OF ENDF/B-VII

Initial ENDF/B-VII produces substantially better agreement with benchmark results than ENDF/B-VI for

- Bare metal spheres (^{233}U, HEU, Pu)
- BIG TEN (10 wt.% U reflected by normal U)
- Water-reflected metal spheres (HEU and Pu)
- Lattices of ^{233}U and LEU fuel pins in water

In addition, the consistency between results for the bare metal spheres and the corresponding Flattop configurations has improved substantially (Flattop configurations consist of a metal sphere reflected by normal uranium)

AREAS OF CONCERN FOR ENDF/B-VII

Data testing with MCNP5 has identified several areas of concern:

- Unresolved resonance region for ^{235}U (Graphite-Moderated Zeus)
- Fast and thermal cross sections for Th (THOR and SB HEU lattice)
- Fast cross sections for ^{237}Np (Np sphere reflected by HEU)
- Fast cross sections for Cu (Unmoderated Zeus)
- Thermal cross sections for ^{233}U and ^{239}Pu (48-inch spheres of solutions)
- Angular scattering distribution for ^{2}H (Heavy-water solutions with high leakage)

NUCLEAR DATA FOR MCNP5 CALCULATIONS

All calculations were performed with continuous-energy nuclear data libraries

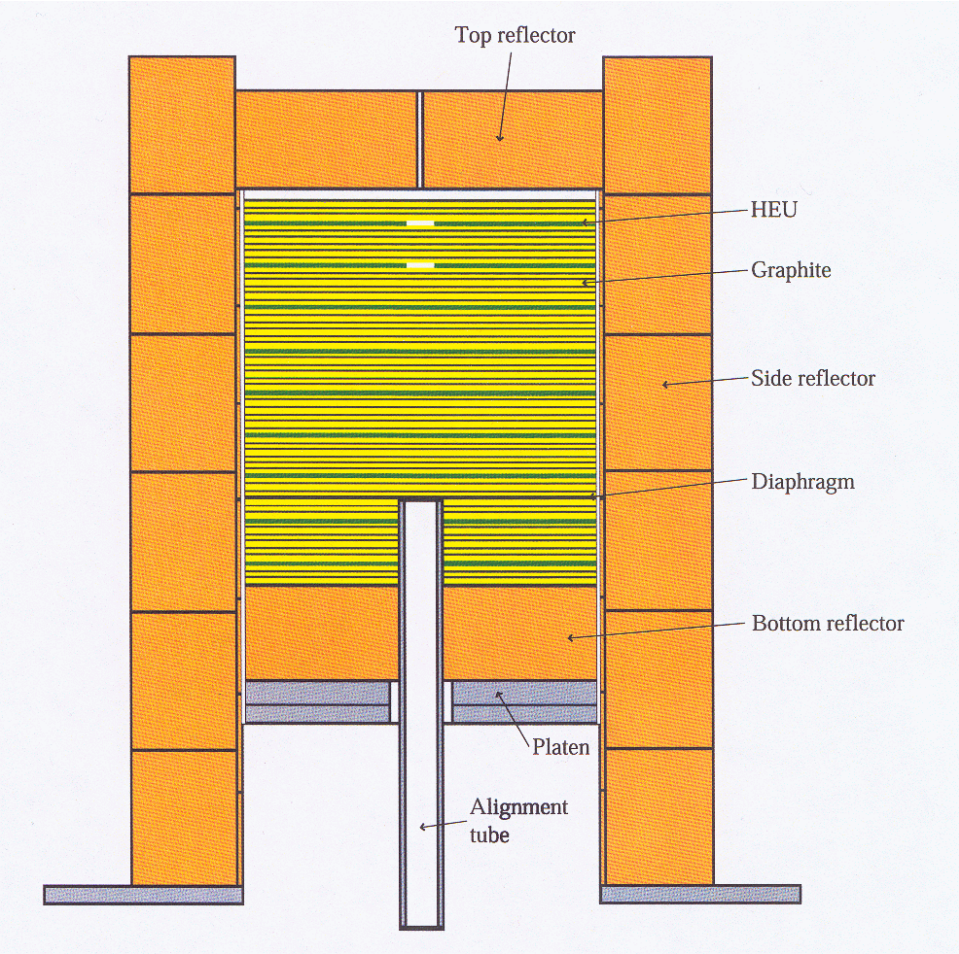
ENDF/B-VI calculations employed the ACTI and ENDF66 nuclear data libraries and the SAB2002 library of thermal scattering laws

Initial ENDF/B-VII calculations employed nuclear data provided by LANL group T-16 for the initial release of ENDF/B-VII

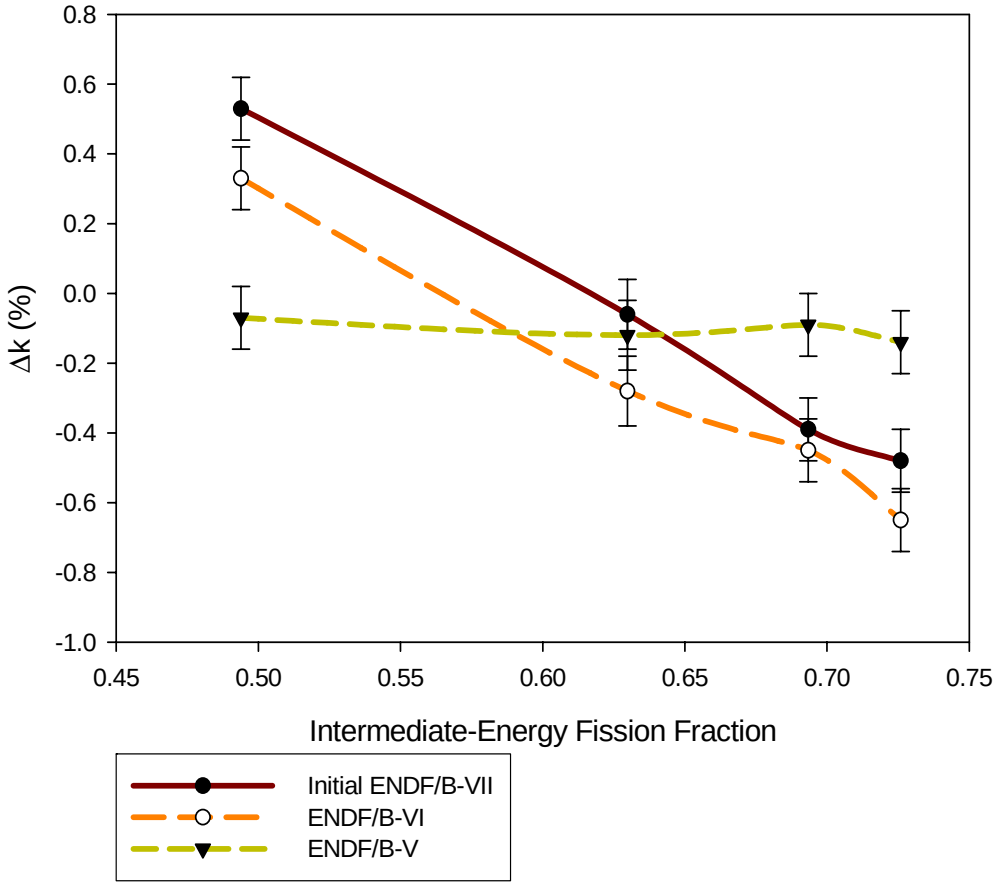
Those ENDF/B-VII data include the uranium isotopes (with new resonance parameters for ^{233}U, ^{235}U, and ^{238}U developed at ORNL), ^{239}Pu, and ^{1}H

ENDF/B-VI nuclear data were retained for all other nuclides in the ENDF/B-VII calculations

ZEUS-2 CONFIGURATION (reasonably representative of others)



ZEUS HEU-GRAPHITE BENCHMARKS



⇒ Cross sections for ^{235}U in the unresolved resonance region should be re-examined

FAST PU METAL BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		Initial ENDF/B-VII	ENDF/B-VI
Jezebel	1.0000 ± 0.0020	0.9998 ± 0.0003	0.9971 ± 0.0003
Jezebel-240	1.0000 ± 0.0020	1.0003 ± 0.0003	0.9980 ± 0.0003
Pu Buttons	1.0000 ± 0.0030	0.9984 ± 0.0003	0.9962 ± 0.0003
Flattop-Pu	1.0000 ± 0.0030	1.0004 ± 0.0003	1.0016 ± 0.0003
THOR	1.0000 ± 0.0006	1.0079 ± 0.0003	1.0057 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

Initial ENDF/B-VII results are within 1 standard deviation for all cases except THOR

THOR consists of central sphere of Pu reflected by Th

⇒ Fast cross sections for Th should be reviewed

THERMAL URANIUM LATTICES

Case	Fuel Type	Benchmark k_{eff}	Calculated k_{eff}	
			Initial ENDF/B-VII	ENDF/B-VI
SB-2½	^{233}U	1.0000 ± 0.0024	0.9988 ± 0.0004	0.9964 ± 0.0004
SB-5	HEU	1.0015 ± 0.0028	0.9957 ± 0.0005	0.9965 ± 0.0005
IEU-CT-02 (3)	IEU	1.0000 ± 0.0030	1.0008 ± 0.0003	1.0004 ± 0.0003
BaW XI (2)	LEU	1.0000 ± 0.0006	1.0000 ± 0.0003	0.9968 ± 0.0003

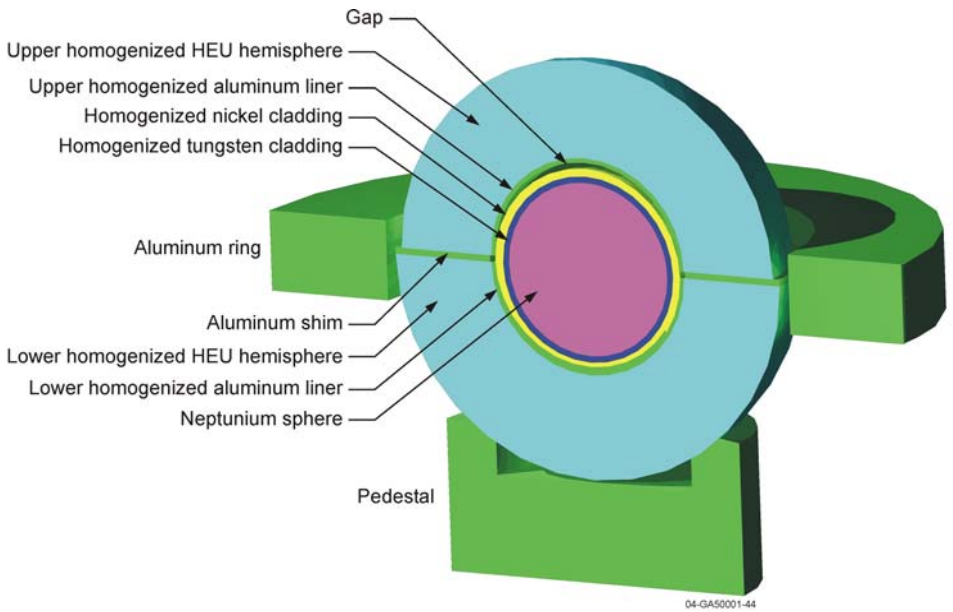
$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

Initial ENDF/B-VII results are within 1 standard deviation for all cases except SB-5

Unlike the others, SB-5 has a buffer region of ThO_2 pins

⇒ Thermal cross sections for Th should be reviewed

NEPTUNIUM SPHERE REFLECTED BY HEU



Benchmark k_{eff}	Calculated k_{eff}	
	Initial ENDF/B-VII	ENDF/B-VI
1.0019 ± 0.0036	0.9924 ± 0.0003	0.9889 ± 0.0002

$$|\Delta k| > 2\sigma$$

⇒ Fast cross sections for ^{237}Np should be reviewed

UNMODERATED ZEUS BENCHMARK

Benchmark k_{eff}	Basic Library	Calculated k_{eff}	
		ENDF/B-VI Cu	ENDF/B-V Cu
1.0012 ± 0.0015	ENDF/B-VII	1.0108 ± 0.0003	1.0001 ± 0.0003
	ENDF/B-VI	1.0080 ± 0.0003	0.9968 ± 0.0003
	ENDF/B-V	1.0088 ± 0.0003	0.9960 ± 0.0003

$|\Delta k| > 2\sigma$

This benchmark has no moderator and therefore has a fast spectrum

Differences between ENDF/B-V and ENDF/B-VI Cu cross sections have little net reactivity impact on previous Zeus benchmarks with graphite moderator, which have intermediate spectra (ENDF/B-VI Cu produces lower capture rate but compensates with higher leakage)

⇒ Fast cross sections for Cu should be reviewed

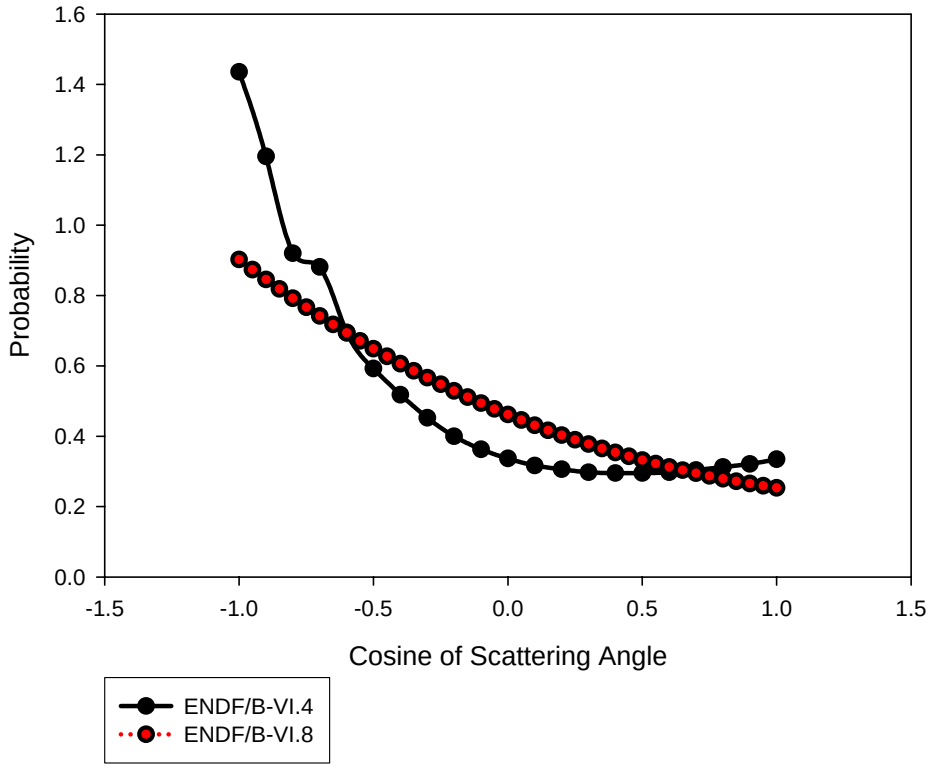
48-INCH SPHERE OF URANYL FLUORIDE OR PLUTONIUM NITRATE SOLUTION

Case	Fuel Type	Benchmark k_{eff}	Calculated k_{eff}	
			Initial ENDF/B-VII	ENDF/B-VI
ORNL-11	^{233}U	1.0006 ± 0.0029	1.0041 ± 0.0002	0.9974 ± 0.0002
ORNL-10	HEU	1.0015 ± 0.0026	0.9989 ± 0.0002	0.9992 ± 0.0002
Pu-ST-09	Pu	1.0000 ± 0.0003	1.0191 ± 0.0002	1.0189 ± 0.0002
			$\sigma < \lvert\Delta k\rvert \leq 2\sigma$	$\lvert\Delta k\rvert > 2\sigma$

Very thermal spectra with very little leakage

⇒ Cross sections for ^{233}U and (especially) ^{239}Pu should be re-examined in the deep thermal range

ENDF/B-VI.4 AND ENDF/B-VI.8 ANGULAR SCATTERING DISTRIBUTIONS FOR ^{1}H AT 1 MeV



ENDF/B-VI.8 distribution has been retained for initial ENDF/B-VII release

RESULTS FOR HEAVY-WATER SOLUTIONS

Benchmark Set	Case	Benchmark k_{eff}	Calculated k_{eff}	
			Initial ENDF/B-VII + ENDF/B-VI.4 ^{2}H	Initial ENDF/B-VII
Reflected Spheres (HEU-SOL-THERM-004)	1	1.0000 ± 0.0033	0.9948 ± 0.0004	0.9839 ± 0.0004
	2	1.0000 ± 0.0036	0.9890 ± 0.0004	0.9795 ± 0.0004
	3	1.0000 ± 0.0039	0.9959 ± 0.0004	0.9862 ± 0.0004
	4	1.0000 ± 0.0046	0.9983 ± 0.0004	0.9892 ± 0.0004
	5	1.0000 ± 0.0052	0.9967 ± 0.0004	0.9877 ± 0.0005
	6	1.0000 ± 0.0059	0.9931 ± 0.0004	0.9844 ± 0.0004
Unreflected Cylinders (HEU-SOL-THERM-020)	1	0.9966 ± 0.0116	1.0013 ± 0.0005	0.9915 ± 0.0005
	2	0.9956 ± 0.0093	1.0066 ± 0.0005	0.9973 ± 0.0005
	3	0.9957 ± 0.0079	1.0152 ± 0.0005	1.0059 ± 0.0005
	4	0.9955 ± 0.0078	1.0129 ± 0.0005	1.0023 ± 0.0005
	5	0.9959 ± 0.0077	1.0176 ± 0.0005	1.0091 ± 0.0005

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

$\Rightarrow$ ^{2}H angular scattering distributions should be reviewed and, if possible, reconciled